1. INTRODUCTION

1.1. BACKGROUND

In May of 1991, the Environmental Protection Agency (EPA) announced a scientific reassessment of the human health and exposure issues concerning dioxin and dioxin-like compounds (56 FR 50903). This reassessment resulted in two reports: a health reassessment document (EPA, 1994), and *Estimating Exposure to Dioxin-Like Compounds*, which expanded upon a 1988 draft exposure report titled, *Estimating Exposure to 2,3,7,8-TCDD* (EPA, 1988). This current *Estimating Exposure to Dioxin-Like Compounds* has expanded to four volumes, as will be discussed below. The health and exposure reassessment documents can be used together to assess potential health risks from exposure to dioxin-like compounds. Numerous public comments were received on these documents and, as well, they were reviewed by EPA's Science Advisory Board in 1995 (EPA, 1995). In a related area, EPA has also discussed the data and methods for evaluating risks to aquatic life from 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD) (EPA, 1993). In 1997, EPA released a workshop review version of Chapter 8 of the Health Reassessment documents, the chapter on dose-response modeling (EPA, 1997). In 1998, EPA released a workshop review version of the sources inventory (EPA, 1998), one of the four volumes of the current Exposure Reassessment Documents.

The purpose of the exposure portion of the dioxin reassessment is threefold: 1) to inventory the known sources of release of dioxins into the environment, 2) to develop an understanding of dioxins in the environment, including fate and transport properties, environmental and exposure media concentrations, background as well as elevated exposures, and temporal trends in exposure, and 3) provide site-specific procedures for evaluating the incremental exposures due to specific sources of dioxin-like compounds.

This current version of the exposure document incorporates changes as a result of comments received on earlier versions of the documents, the SAB review in 1995, the workshop held in 1998 on the sources inventory, and a wealth of new information on dioxins available in the open literature.

The exposure document is presented in four volumes. Following is a summary of the material contained in each of the four volumes:

Volume I - Executive Summary

This volume includes summaries of findings from Volumes II, III, and IV. It also includes a unique section on research needs and recommendations for dioxin-like compounds.

Volume II - Inventory of Sources of Dioxin in the United States

This volume presents the inventory of known sources of dioxin release into the US environment. This inventory is presented for two time frames, represented by the years 1987 and 1995. Ongoing releases into air, water, and soil are quantified where possible. Also, estimates of release from "reservoir" sources of dioxins, such as soils or pentachlorophenol-treated utility poles, are presented.

Volume III - Properties, Environmental Levels, and Background Exposures

This volume presents and evaluates information on the physical-chemical properties, environmental fate, environmental and exposure media levels, background and elevated human exposures, and temporal trends of dioxin-like compounds in the US environment during the 20th century. It summarizes and evaluates relevant information obtained from published literature searches, EPA program offices and other Federal agencies, and published literature. From these data sources, this volume generates important quantities including exposure media concentrations, and average as well as elevated exposure levels for US citizens. The data contained in this volume are expected to be current through 1998 with some new information published during 1999.

Volume IV - Site-Specific Assessment Procedures

This volume presents procedures for evaluating the incremental impact from sources of dioxin release into the environment. The sources covered include contaminated soils, stack emissions, and point discharges into surface water. This volume includes sections on: exposure parameters and exposure scenario development; stack emissions and atmospheric transport modeling; aquatic and terrestrial fate, and food chain modeling; demonstration of methodologies; and uncertainty evaluations including exercises on sensitivity analysis and model validation, review of Monte Carlo assessments conducted for dioxin-like compounds, and other discussions. The data contained in this volume are current through 1998 with some new information published during 1999.

1.2. DESCRIPTION OF DIOXIN-LIKE COMPOUNDS

This document addresses compounds in the following chemical classes: polychlorinated dibenzo-p-dioxins (PCDDs or CDDs), polychlorinated dibenzofurans (PCDFs or CDFs), and

polychlorinated biphenyls (PCBs). The CDDs include 75 individual compounds, and CDFs include 135 different compounds. These individual compounds are technically referred to as congeners. Only 7 of the 75 congeners of CDDs are thought to have dioxin-like toxicity; these are ones with chlorine substitutions in, at least, the 2, 3, 7, and 8 positions. Only 10 of the 135 possible congeners of CDFs are thought to have dioxin-like toxicity; these also are ones with substitutions in, at least, the 2, 3, 7, and 8 positions. There are 209 PCB congeners. Only 13 of the 209 congeners are thought to have dioxin-like toxicity; these are PCBs with four or more chlorines with just one or no substitution in the ortho position. These compounds are sometimes referred to as coplanar, meaning that they can assume a flat configuration with rings in the same plane. Similarly configured polybrominated biphenyls are likely to have similar properties; however, the data base on these compounds, with regard to dioxin-like activity, have been less extensively evaluated.

The physical/chemical properties of each congener vary according to the degree and position of chlorine substitution. The chlorinated dibenzodioxins and dibenzofurans are tricyclic aromatic compounds with similar physical and chemical properties, and both classes are similar structurally. Certain PCBs (the so-called coplanar or mono-ortho coplanar congeners) are also structurally and conformationally similar. The most widely studied of these compounds is 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD). This compound, often called simply dioxin, represents the reference compound for this class of compounds. The structure of 2,3,7,8-TCDD and several related compounds is shown in Figure 1-1.

1.3. TOXICITY EQUIVALENCY FACTORS

The dioxin-like compounds are often found in complex mixtures. For risk assessment purposes, a toxicity equivalency procedure was developed to describe the cumulative toxicity of these mixtures. This procedure involves assigning individual toxicity equivalency factors (TEFs) to the 2,3,7,8 substituted CDD and CDF congeners (the sum of these two abbreviated CDD/F in this document) and to selected coplanar and mono-ortho PCBs (the sum of the three groups often abbreviated CDD/F/PCB). TEFs are estimates of the toxicity of dioxin-like compounds relative to the toxicity of 2,3,7,8-TCDD, which is assigned a TEF of 1.0. Calculating the toxic equivalency (TEQ) of a mixture involves multiplying the concentration of individual congeners by their respective TEF. The sum of the TEQ concentrations for the individual congeners is the TEQ concentration for the mixture. This is described mathematically as follows:

$$TEQ \cong \sum_{i-n}\left(Congener_i \times TEF_i\right) + \left(Congener_j \times TEF_j\right) + ...\left(Congener_n \times TEF_n\right)$$

On the most basic level, TEFs compare the potential toxicity of each dioxin-like compound comprising the mixture to the well-studied and understood toxicity of 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD), the most toxic member of the group. To assign TEF values, scientist have reviewed the toxicological databases along with considerations of chemical structure, persistence, and resistance to metabolism. Since 1989, three different TEF schemes have been developed and used for evaluating the TEQ of mixtures of CDDs, CDFs and dioxin-like PCBs. A problem arises in that past and present quantitative exposure and risk assessments may not have clearly identify which of three TEF schemes were used to estimate the TEQ. This Dioxin Exposure Reassessment document will adopt a uniform TEQ nomenclature that clearly distinguishes between the three major TEF schemes. The following presents a taxonomy of TEQ.

1. I-TEQ$_{DF}$

Described by EPA in 1989 (EPA, 1989), this procedure assigns TEFs only for the 7 dioxin (CDDs) and 10 furans (CDFs). The TEF values for the I-TEQ$_{DF}$ are shown in Table 1 below. Note that the scheme does not include dioxin-like PCBs. The nomenclature for this scheme is I-TEQ$_{DF}$, where 'I' represents 'International', TEQ represents the 2,3,7,8-TCDD Toxic Equivalence of the mixture, and the subscript DF indicates that only dioxins (Ds) and furans (Fs) are included in the TEF scheme. In this document, this will often be shortened to I-TEQ without the subscripts where it is understood, in the context of the discussion, that the TEQ mixture refers to both dioxins and furans. There may also be occasion to describe I-TEQ$_{D}$ or I-TEQ$_{F}$, when it is only desired to denote the TEQ concentrations of dioxins only or furans only in the mixture.

2. TEQ$_{DFP}$-WHO$_{94}$

In 1994, the World Health Organization (WHO) added 13 dioxin-like PCBs to the TEF scheme for dioxins and furans (Ahlborg et al., 1994). However, no changes were made to the TEFs for dioxins and furans. The nomanclature for this TEF scheme is TEQ$_{DFP}$-WHO$_{94}$, where TEQ represents the 2,3,7,8-TCDD Toxic Equivalence of the mixture, and the subscript DFP indicates that dioxins (Ds) furans (Fs) and dioxin-like PCBs (P) are included in the TEF scheme. The subscript 94 following WHO displays the year changes were made to the TEF scheme. As in

the above scheme, there may be occasions where the DFP subscript can be tailored to the context of the discussion. For example, to describe the TEQ concentration of only the dioxin-like PCBs of a mixture using this WHO 1994 scheme, the nomenclature would read, TEQ_{P}-WHO_{94}. For a mixture containing dioxins, furans, and coplanar PCBs, the full TEQ_{DFP}-WHO_{94} would be used. There would no occasion for TEQ_{DF}-WHO_{94}, since the TEFs for CDD/Fs did not change in the 1994 WHO designations - TEQ concentrations using the international TEFs for CDD/Fs would be described, as noted above, as I-TEQ. Table 2 displays the TEFs for the dioxin-like coplanar PCBs, developed in 1994 by the World Health Organization.

3. TEQ_{DFP}-WHO_{98}

In 1998, the WHO re-evaluated the previously established TEFs for dioxins, furans, and dioxin-like PCBs (Van den Berg, et al., 1998). Changes were made to the 1989 International TEFs for dioxins and furans, as well as to the 1994 TEFs for coplanar PCBs. The nomanclature for this TEF scheme is TEQ_{DFP}-WHO_{98}, where TEQ represents the 2,3,7,8-TCDD Toxic Equivalence of the mixture, and the subscript DFP indicates that dioxins (Ds) furans (Fs) and dioxin-like PCBs (P) are included in the TEF scheme. The subscript 98 following WHO displays the year changes were made to the TEF scheme. As noted before, the subscripts D, F, and P can be used in various combinations to denote TEQ concentrations for mixtures including only CDD/Fs (TEQ_{DF}-WHO_{98}), only PCBs (TEQ_{P}-WHO_{98}), or all three (TEQ_{DFP}-WHO_{98}). Table 3 displays the TEF scheme for the TEQ_{DFP}-WHO_{98}. Note that the changes to the TEFs for dioxins and furans are as follows:

- For 1,2,3,7,8-PeCDD, the new WHO TEF is 1 and the I-TEF is 0.5;
- For OCDD, the new WHO TEF is 0.0001 and the I-TEF is 0.001; and
- For OCDF, the new WHO TEF is 0.0001 and the I-TEF is 0.001.

Note that the changes to the TEFs for dioxin-like PCBs (Ps) are as follows:

- For PCB 77, the new TEF is 0.0001;
- The Addition of PCB 81 (i.e., 3,4,4',5-TCB); and
- For the two di-ortho substituted HpCBs in the 1994 TEF scheme (i.e,. PCBs 170 and 180), TEFs of zero have been assigned in the new WHO TEF scheme.

1.4. OVERALL COMMENTS ON THE USE OF VOLUME IV OF THE DIOXIN EXPOSURE DOCUMENT

Users of the dioxin exposure document should recognize the following:

1. This document does not present detailed procedures for evaluating multiple sources of release. However, it can be used in two ways to address this issue. Incremental impacts estimated with procedures in Volume IV can be compared to background exposure estimates which are presented in Volume III. This would be a way of comparing the incremental impact of a specific source to an individual's total exposure otherwise. Assuming the releases from multiple sources behave independently, it is possible to model them individually and then add the impacts. For example, if several stack emission sources are identified and their emissions quantified, and it is desired to evaluate the impact of all sources simultaneously, then it is possible with ISCST3 to model each stack emission source individually and then sum the concentrations and depositions at points of interest in the surrounding area.

2. The demonstration of the site-specific procedures presented in this exposure document best serve as general examples for evaluating exposures to dioxin-like compounds, rather than specific assessments. This demonstration scenarios in Chapter 5 of this document were not generated for purposes of supporting any specific regulation. Rather, they were only intended to demonstrate the procedure described earlier in Chapters 2 through 4. Certainly, the goal of developing “high end” and “central” is consistent with Agency policy, and even assignment of many of the exposure and fate parameters can be adopted for other assessments. Therefore, assessors may find even the specifics of the demonstration scenarios useful for other purposes.

3. The understanding of the exposure to dioxin-like compounds continues to expand. Despite being one of the most studied groups of organic enivronmental contaminants, new information is generated almost daily about dioxin-like compounds. This document is considered to be current through 1998, with some information published during 1999 included as well. Section IV of Volume I, Executive Summary, discusses research needs for dioxin exposure evaluation.

1.5. NOTES ON THE USE OF PROCEDURES IN VOLUME IV

Numerous parameter values are used in this document and it is important to understand their degree of "endorsement" by EPA. The parameters can be divided into the following four classes for purposes of addressing this issue:

1) **First Order Defaults:** As defaults, these parameters are independent of site specific characteristics and can be used for any assessment. Also, as first order defaults, it is felt that the

values selected for the demonstration scenarios carry a sufficient weight of evidence from current literature such that these values are recommended for other assessments. Several of the chemical specific parameters, such as the Henry's Constant, H, and the organic carbon partition coefficient, Koc, fall into this category. The qualifier above, "current literature", indicates that new information could lead to changes in these values.

2) **Second Order Defaults:** Like the above category, these parameters are judged to be independent of site specific characteristics. However, unlike the above category, the current scientific weight of evidence is judged insufficient to describe values selected for demonstration purposes as first order defaults. Parameters of principal note in this category are the bioconcentration parameters specific to the chemicals, such the Biota Sediment Accumulation Factor, or BSAF. This parameter translates a bottom sediment concentration to a fish tissue concentration. The science is evolving for this parameter, including thought on the extent to which BSAFs generated for one species at one site can be generalized to other sites and/or species, the differences in BSAF between column and bottom feeders, the differences between past and ongoing contamination, and so on. Users should carefully review the justification for the SOD values selected for the demonstration scenarios before using the same values.

3) **Site Specific:** These parameters should or can be assigned values based on site-specific information. The information provided on their assignment for the demonstration of methodologies in this document can be useful where site specific information is unavailable. A key class of site specific are the source strength terms - the soil concentrations, effluent discharge rates, and stack emission rates. Others include physical properties (organic carbon contents of soil and sediment, climate variables, areas, distances, and volumes) and parameters for bioconcentration algorithms (yields of vegetations, cattle raising practices, fish lipid contents).

4) **Exposure Parameters:** The exposure parameters have not been categorized as have the contaminant fate and transport/transfer parameters. Assignment of these values are critical as Lifetime Average Daily Dose (LADD) estimates are linearly related to parameter assignments - doubling exposure duration assumptions double LADDs, and so on. Some exposure parameters are appropriately described as first order defaults. These include: lifetime, body weights, water ingestion rates, inhalation rates, and an exposure duration for a childhood pattern of soil ingestion. All of the other exposure parameters are better described as either second order defaults or site specific parameters. All exposure parameters were developed based on information and recommendations in EPA's *Exposure Factors Handbook* (EPA, 1997) and *Dermal Exposure Assessment: Principles and Applications* (EPA, 1992).

The end products of the exposure assessment procedures presented in this document are estimates of potential dose expressed in mass (pg, ng, etc.) of dioxin-like compound/body weight (usually kg)-day. The procedures for converting these dose estimates to risk estimates, both cancer and non-cancer, are described in Chapter 2 and demonstrated in Chapter 5.

The scope of each chapter in Volume III is summarized below.

Chapter 2, Estimating Exposure and Risks, presents overall framework for conducting exposure assessments. It provides procedures for identifying exposure pathways, estimating contact rates and resulting exposure levels. Approaches for defining exposure scenarios are presented. Procedures for converting exposure dose to lifetime cancer risk estimates are provided, and procedures for evaluating non-cancer risk are also discussed.

Chapter 3, Evaluating Atmospheric Releases of Dioxin-Like Compounds from Combustion Sources, provides procedures to estimate the emission rates of dioxin-like compounds from combustion processes and further atmospheric transport modeling procedures from the stack to the surrounding land surface. This chapter describes and demonstrates the use of the ISCST3 model on a hypothetical incinerator and lists the associated atmospheric dispersion and deposition estimates from that model exercise.

Chapter 4, Estimating Exposure Media Concentrations, provides procedures for estimating concentrations of the dioxin-like compounds in exposure media (soil, air, water, biota) resulting from soil contamination, effluent discharges, and stack emissions.

Chapter 5, Demonstration of Methodology, develops hypothetical scenarios and generates exposure and risk estimates to demonstrate the methodologies of this document.

Chapter 6, User Considerations, discusses key issues for users of the methodologies. All model parameters are listed and categorized according to the scheme noted above. Sensitivity analysis is conducted on the algorithms estimating exposure media concentrations. An exercise on estimating the releases from a bounded area of soil contamination is presented. The purpose of this exercise is to determine whether a reservoir of soil contamination would be depleted prior to an assumed duration of exposure.

Chapter 7, Model Comparisons and Validations, presents extensive information aimed at gaining confidence and establishing credibility for the use of the fate models of this assessment to predict the fate, movement, and resulting exposure media concentrations near sources of dioxin release. One section of this chapter presents alternate fate models, and where possible, generates results from these models to compare with results from the models selected for this assessment. The second major section presents several model validation exercises, where the

models are paramterized to predict exposure media concentrations, and the results are compared with appropriate real world observations.

Chapter 8, Uncertainty, discusses the sources and possible magnitude of uncertainty in the exposure assessment procedures. Uncertainty and variability of fate and transport, and exposure parameters, are discussed. Monte Carlo and similar numerical methods to quantify variability and uncertainty are discussed, and several literature examples of these types of exercises conducted for dioxin-like compounds are summarized.

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Table 1-1. The TEF scheme for I-TEQ_{DF}

Dioxin (D) Congener	TEF	Furan (F) Congener	TEF
2,3,7,8-TCDD	1.0	2,3,7,8-TCDF	0.1
1,2,3,7,8-PeCDD	0.5	1,2,3,7,8-PeCDF	0.05
1,2,3,4,7,8-HxCDD	0.1	2,3,4,7,8-PeCDF	0.5
1,2,3,6,7,8-HxCDD	0.1	1,2,3,4,7,8-HxCDF	0.1
1,2,3,7,8,9-HxCDD	0.1	1,2,3,6,7,8-HxCDF	0.1
1,2,3,4,6,7,8-HpCDD	0.01	1,2,3,7,8,9-HxCDF	0.1
OCDD	0.001	2,3,4,6,7,8-HxCDF	0.1
		1,2,3,4,6,7,8-HpCDF	0.01
		1,2,3,4,7,8,9-HpCDF	0.01
		OCDF	0.001

Table 1-2. The TEF scheme for dioxin-like coplanar PCBs, as determined by the World Health Organization in 1994

Chemical Structure	IUPAC Number	TEF
3,3',4,4'-TeCB	PCB-77	0.0005
2,3,3',4,4'-PeCB	PCB-105	0.0001
2,3,4,4',5-PeCB	PCB-114	0.0005
2,3',4,4',5-PeCB	PCB-118	0.0001
2',3,4,4',5-PeCB	PCB-123	0.0001
3,3',4,4',5-PeCB	PCB-126	0.1
2,3,3',4,4',5-HxCB	PCB-156	0.0005
2,3,3',4,4',5'-HxCB	PCB-157	0.0005
2,3',4,4',5,5'-HxCB	PCB-167	0.00001
3,3',4,4',5,5'-HxCB	PCB-169	0.01
2,2',3,3',4,4',5-HpCB	PCB-170	0.0001
2,2',3,4,4',5,5'-HpCB	PCB-180	0.00001
2,3,3',4,4',5,5'-HpCB	PCB-189	0.0001

Table 1-3. The TEF scheme for TEQ_{DFP}-WHO_{98}

Dioxin Congeners	TEF	Furan Congeners	TEF
2,3,7,8-TCDD	1.0	2,3,7,8-TCDF	0.1
1,2,3,7,8-PeCDD	1.0	1,2,3,7,8-PeCDF	0.05
1,2,3,4,7,8-HxCDD	0.1	2,3,4,7,8-PeCDF	0.5
1,2,3,6,7,8-HxCDD	0.1	1,2,3,4,7,8-HxCDF	0.1
1,2,3,7,8,9-HxCDD	0.1	1,2,3,6,7,8-HxCDF	0.1
1,2,3,4,6,7,8-HpCDD	0.01	1,2,3,7,8,9-HxCDF	0.1
OCDD	0.0001	2,3,4,6,7,8-HxCDF	0.1
		1,2,3,4,6,7,8-HpCDF	0.01
		1,2,3,4,7,8,9-HpCDF	0.01
		OCDF	0.0001

Chemical Structure	IUPAC Number	TEF
3,3',4,4'-TeCB	PCB-77	0.0001
3,4,4',5-TCB	PCB-81	0.0001
2,3,3',4,4'-PeCB	PCB-105	0.0001
2,3,4,4',5-PeCB	PCB-114	0.0005
2,3',4,4',5-PeCB	PCB-118	0.0001
2',3,4,4',5-PeCB	PCB-123	0.0001
3,3',4,4',5-PeCB	PCB-126	0.1
2,3,3',4,4',5-HxCB	PCB-156	0.0005
2,3,3',4,4',5'-HxCB	PCB-157	0.0005
2,3',4,4',5,5'-HxCB	PCB-167	0.00001
3,3',4,4',5,5'-HxCB	PCB-169	0.01
2,3,3',4,4',5,5'-HpCB	PCB-189	0.0001

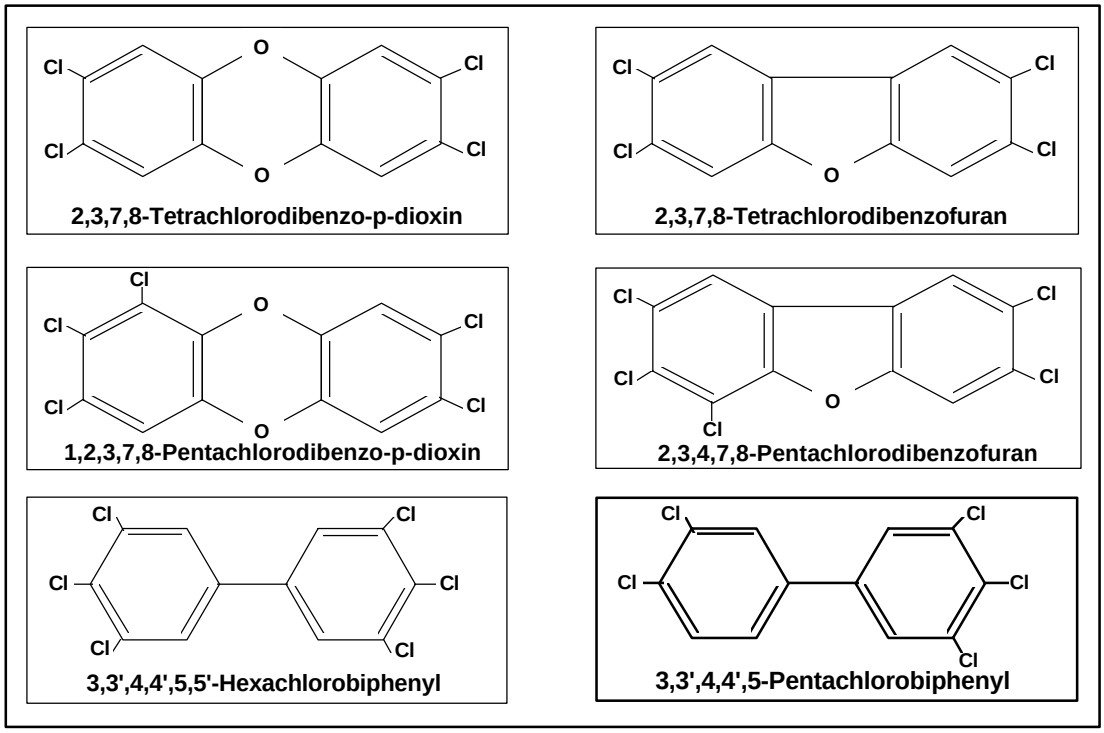

Figure 1-1. Chemical structure of 2,3,7,8-TCDD and related compounds